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Using MODIS surface albedo and TOMS data for improving the description of air quality model

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Abstract

Accurate representations of photolysis rates are crucial in photochemical modeling. These reaction rates determine the formation of radicals that drive tropospheric O_3 and secondary aerosol production. For this, correct calculation of spatially and temporally resolved actinic flux is needed. Actinic flux is affected by earth's surface albedo, amount of column ozone, aerosols, clouds, and other trace gases that affect the attenuation of near ultraviolet and visible light. In the Community Multiscale Air Quality Modeling System (CMAQ), actinic flux is calculated by the delta-Eddington two-stream radiative transfer model (Joseph et al., 1976). Current surface albedo is parameterized as eight discrete values that depend only on wavelengths (Demerjian et al., 1980), with no temporal or spatial variability. The vertical ozone profiles are set by interpolating seasonal profiles from a default input file, without considering inter-annual, seasonal, or monthly variability.

Remotely sensed satellite data can provide synoptic and geospatial information with high spatial and temporal resolution to ground-based air quality data and modeling (Engel-Cox et al., 2004). In this study, we characterize spatial and temporal variability in surface albedo for our modeling domain in the Central California region, using the Moderate Resolution Imaging Spectroradiometer (MODIS) Bidirectional Reflectance Distribution Function (BRDF)/Albedo product. Temporal trends in the amount and variability of total column ozone are also computed using the Total Ozone Mapping Spectrometer (TOMS) data. We report the results of photochemical simulations and sensitivity studies using the CMAQ modeling system for the Central California region to further quantify the impact of albedo and total column ozone on photolysis rates and ozone production.

Photolysis Rates in CMAQ

Photolysis Rate Preprocessor (JPROC) is one of the major processors in CMAQ. It is used to calculate chemical mechanism-specific clear sky photolysis rates (J_i) at fixed altitudes, hour angles, and latitude bands (EPA, 1999).

$$J_i = \int_{\lambda_1}^{\lambda_2} F(\lambda)\sigma_i(\lambda)\phi_i(\lambda)d\lambda$$

where, $F(\lambda)$ is the actinic flux (photons cm^{-2} min^{-1} nm^{-1}), $\sigma_i(\lambda)$ the absorption cross section for the molecule undergoing photodissociation (cm^2 molecule^{-1}), $\phi_i(\lambda)$ the quantum yield of the photolysis reaction (molecules photon^{-1}), and λ the wavelength (nm). $\sigma_i(\lambda)$ and $\phi_i(\lambda)$ are functions of wavelength and unique to species and reactions, measured through laboratory experiments. $F(\lambda)$ is a radiometric quantity that measures the spectral radiance integrated over all solid angles per unit area. It changes with time of day, location, latitude, altitude, and season, and is governed by the astronomical and geometrical relationships between the sun and the earth.

The current approach taken for computing the actinic flux in the CMAQ framework follows the delta-Eddington two-stream radiative transfer model (Joseph et al., 1976; Toon et al., 1989). A description of the extraterrestrial radiation, aerosol, ozone absorption, oxygen absorption in the Schumann-Runge Bands, Rayleigh scattering and surface albedo are provided to the radiation model (EPA, 1999).

The problems in current CMAQ include: 1) The albedo data given by Demerjian et al. (1980), as a function of wavelength, are used in the current version of JPROC. They are the discrete values in eight spectral bands, with no temporal or spatial variability (Table 1).
2) The vertical ozone profiles in CMAQ are set by interpolating seasonal profiles from a default input file, without considering inter-annual, seasonal, monthly, or spatial variability. The initial phase of our current study is directed toward improving the description of albedo, and ozone parameters in CMAQ.

Table 1 Albedo in CMAQ/JPROC's subroutine SETALB

Wavelength(nm)	Albedo
<400	0.05
400-450	0.06
450-500	0.08
500-550	0.10
550-600	0.11
600-640	0.12
640-660	0.135
>660	0.15

Table 2 The spectral bands in MODIS

Band	Wavelength(nm)
Blue	459-479
Green	545-565
Red	620-670
NIR	841-876
NIR	1230-1250
NIR	1628-1652
NIR	2105-2155
VIS-BB	300-700
NIR-BB	700-5000
SW-BB	300-5000

Surface Albedo from MODIS

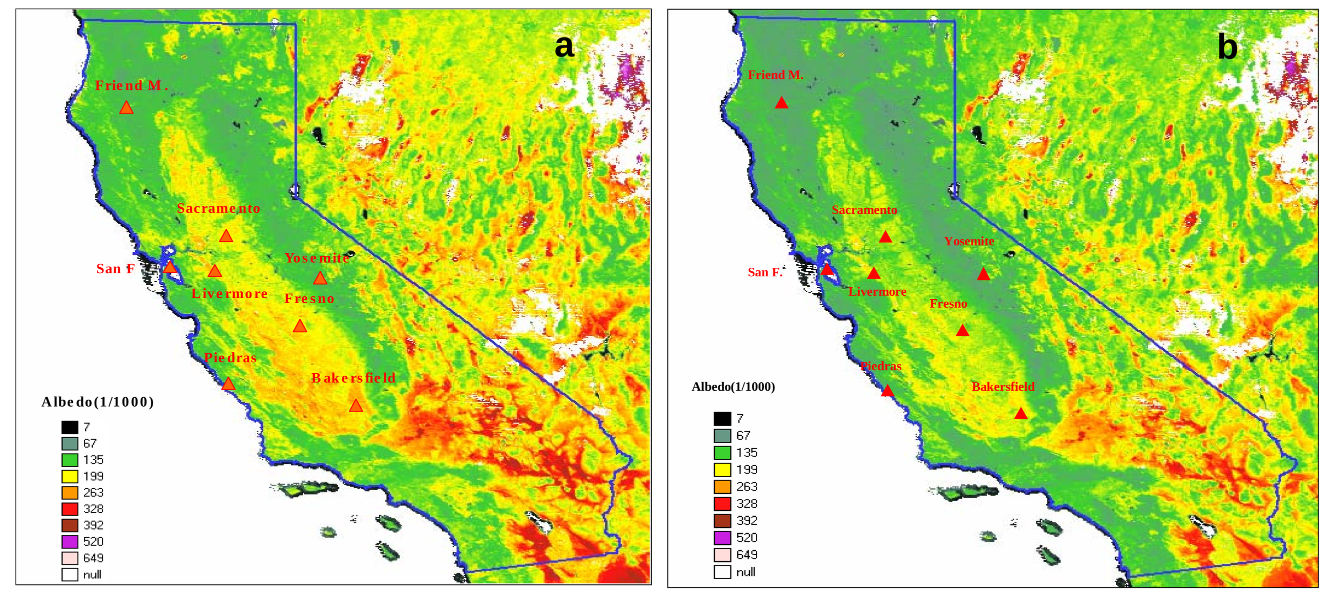


Figure 1 Surface Albedo from MODIS for 07/27/2000 to 08/11/2000.
a) White-sky albedo;
b) Black-sky albedo at solar noon.
Wavelength: 0.3-5.0 µm

The MODIS Albedo 16-Day L3 Global 1km SIN Grid product, MOD43B3, provides black-sky albedo (at the mean solar zenith angle at local solar noon) and white-sky albedo (Figure 1). Each pixel (1km×1km) has one albedo value according to BRDF parameters in seven spectral bands and three broadbands (Table 2). For the MODIS BRDF/Albedo products, the black-sky albedo (directional hemispherical reflectance) is defined as albedo in the absence of a diffuse component and is a function of solar zenith angle. The white-sky albedo (bihemispherical reflectance) is defined as albedo in the absence of a direct component when the diffuse component is isotropic. Black-sky albedo and white-sky albedo mark the extreme cases of completely direct and completely diffuse illumination. Actual albedo is a value which is interpolated between these two as a function of the fraction of diffuse skylight which is itself a function of the aerosol optical depth [Lucht, et al., 2000].

Comparison of Albedos from MODIS and CMAQ

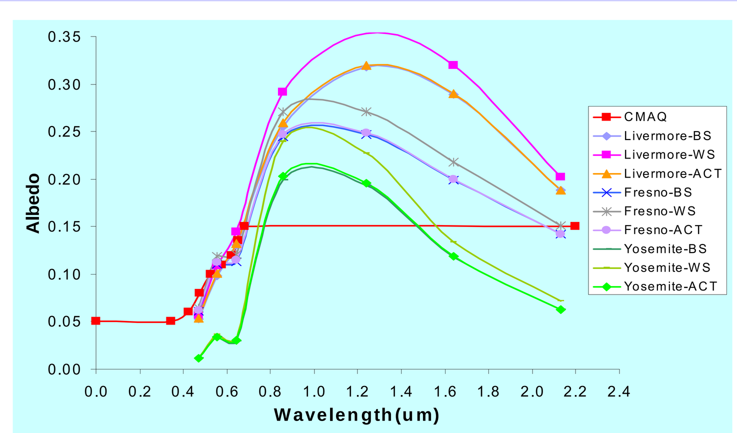
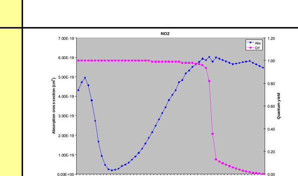
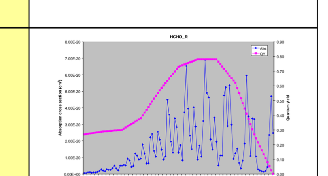
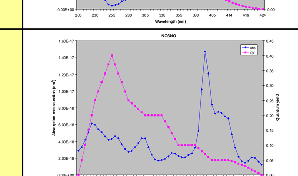
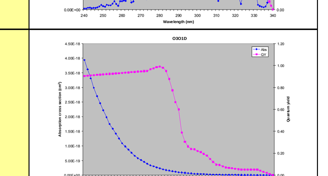
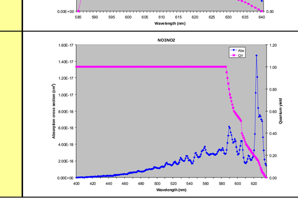
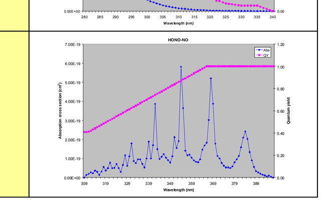


Figure 2 Comparison of Black-sky, White-sky and Actual Albedo at different locations with CMAQ data.

Figure 2 shows the difference of the black-sky albedo at solar noon zenith angle, white-sky albedo and actual albedo at different wavelengths and at different locations on July 27, 2000. In the bands of wavelength less than 700nm (visible and near UV), the black-sky albedo, white-sky albedo and actual-albedo are very similar. The difference between black-sky and white-sky albedo at most places is less than 0.01, with a range from 0 to 0.014. The ratios of differences are less than 10%, with a range from 3.11% to 9.84%. The MODIS albedo in urban regions is close to the CMAQ data.

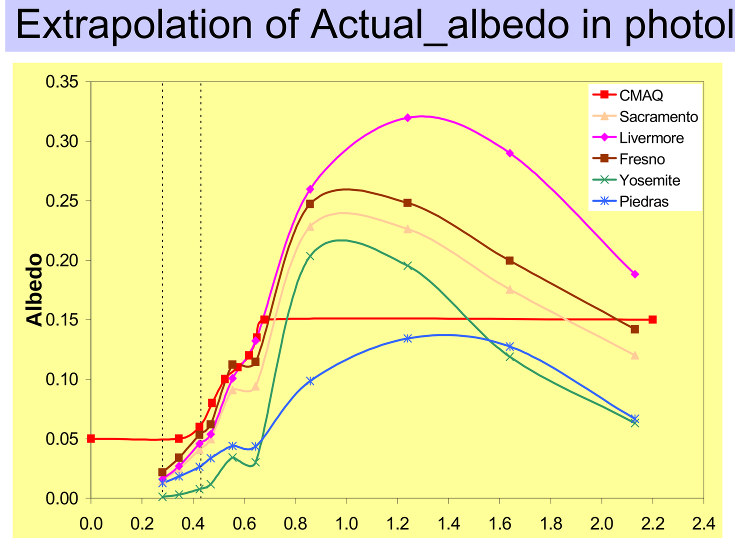
Photolysis reactions in CMAQ

Table 3 Absorption cross sections and quantum yields for the photolysis reactions (adapted from Carter, 2000)

Reaction	Wavelength (nm)	Absorption cross section & Quantum yield	Reaction	Wavelength (nm)	Absorption cross section & Quantum yield
$NO_2 = NO + O^3P$	205-424		$HCHO=2*HO_2+CO$	240-340	
$NO_3 = NO + O_2$	585-640		$O_3 = O^1D + O_2$	280-340	
$NO_3 = NO_2 + O^3P$	400-635		$HONO = HO + NO$	309-400	

We adopt the SAPRC99 chemical mechanism (Carter, 2000) in our CMAQ runs. Examples of photolysis reactions with the absorption cross sections and quantum yields are listed in Table 3. Most of photolysis reactions take place within the wavelength less than 700 nm, especially less than 400nm.

Extrapolation of Actual_albedo in photolysis region



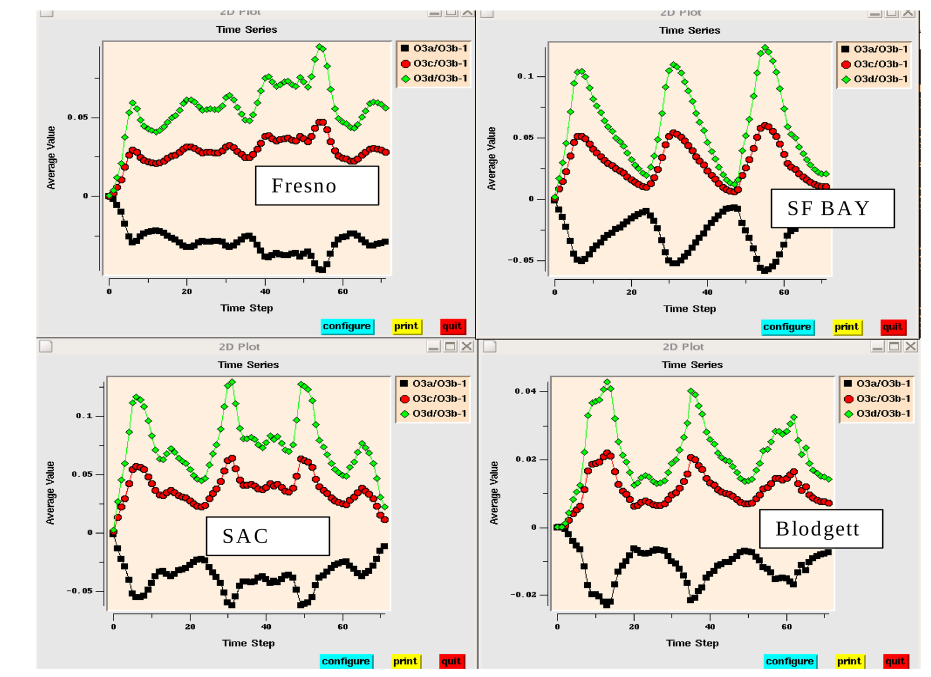
Since the UV band is very important for the photochemistry, we extrapolate the actual-albedo from MODIS spectra to the photolysis region (280-430nm) using a power law: ALB=aλ^b. The extrapolation results show the Actual_albedo in the photolysis region are all less than 0.05 and of similar numerical value, which is verified by the literature (Figure 3). The albedo in the UV for most snow free surfaces ranges about from 0.01 (grassland) to 0.15 (limestone) [Blumthaler and Ambach, 1988]. The difference between urban and rural areas decrease as the wavelengths decrease.

Figure 3 Extrapolation of Actual_albedo in Photolysis region.

Perturbation and simulation in CMAQ

Surface albedo is an influential parameter on ozone production. We performed brute force perturbations by zeroing out, doubling, and tripling the surface albedo in different CMAQ simulations. The results showed that the ozone changes due to changes in the albedo varied linearly. Tripling the albedo caused about 5 ppb increase in the modeled ozone in the valley. Relative increases in ozone is larger at more polluted sites (~5% v.s. ~2%), with the absolute values of 5 ppb v.s. 1 ppb, which is likely caused by more efficient chain reactions (Figure 4).

Since we can only obtain >400nm albedo data from MODIS, we also did perturb-albedo runs for different wavelength: (1) double albedo only for wavelength <400nm; (2) double albedo only for wavelength >400nm. The ozone sensitivity is about five times larger at lower wavelengths.



O3a: Zero; O3b: Original; O3c: Double; O3d: Triple

Figure 4 Relative difference of ozone concentration in perturbed runs at Fresno, San Francisco Bay (SFB), Sacramento (SAC), and Blodgett.

Total Column Ozone from TOMS

Currently, the vertical ozone profiles are set by interpolating seasonal profiles from a default input file, without considering inter-annual, seasonal, or monthly variability. Using the Total Ozone Mapping Spectrometer (TOMS) data from 1979 to 2005, we characterized the temporal trends in the ozone column and its variability for our modeling domain in the Central California region.

Temporal variation of Total Column Ozone

The daily averages of total column ozone (TCO) in California show a seasonal variation with larger values in spring (March 22 to June 21), lower values in summer and fall, and a large day-to-day variability (Figure 5-a). The systematic seasonal variation is due to the general circulation in the stratosphere. The day-to-day variation is related to the meteorological conditions. Monthly means of TCO decrease with time. Seasonal amplitudes decrease with time, which is related to the absolute value of the ozone concentration. Yearly means of TCO in California decrease with time for the period 1979 to 2005 (Figure 5-b), which is similar to the global mean total column ozone.

Most air quality modeling studies with CMAQ are conducted for the Eastern United States; thus we compared the total column ozone for our modeling domain in Central California to one for the Eastern US to determine the impact of using an Eastern TCO parameterization on model performance in California. The long term trends of yearly average total ozone in these two regions are similar, and decrease with time; however, the daily and monthly average TCO in year 2000, of concern in our study, are quite different in California and the Eastern US, especially in the Spring.
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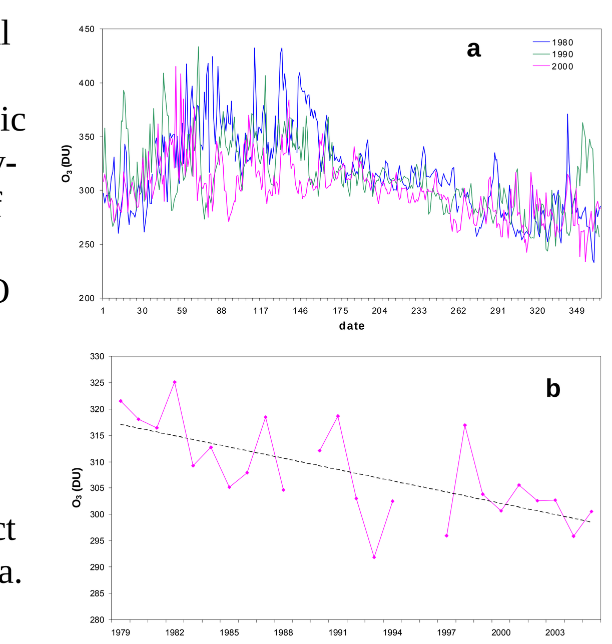

Figure 5 Time series of total column ozone in Central California. a) daily means; b) yearly means.

Comparison of TCO from TOMS and CMAQ

In order to compare total column ozone from TOMS with the CMAQ default data, we computed the scaling factor of column ozone for latitude bands 30 and 40. The maximum change for most cases in 2000, from Julian date 206 to 220, is a 5% increase compared with the default data in CMAQ. J values computed after adjusting column ozone by TOMS data indicate a maximum change of 6% at all altitudes at latitude 30, which occurs at larger hour zenith angles. Relative to the perturbed-albedo study, this difference corresponds to a 3-4 ppb difference in ozone concentrations.

Conclusions

- **Compared with the CMAQ representation of albedo, MODIS surface albedo products indicate substantial temporal and spatial variations, which are influential for ozone production.**
- **Ozone production increase with surface albedo and the absolute increase is larger at more polluted sites (~4ppb v.s. ~1ppb) with relative increases of ~5% v.s. ~2% at the same sites.**
- **Total column ozone from TOMS averaged over different time periods decreases in California over the longer term (1979 to 2005) as it does in the East Coast and globally. Annual modeling as is required for PM and visibility would be more affected by these variations than seasonal ozone modeling. In general, it would be better to include actual profile data as model input for specific time periods and regions of the country.**
- **After adjusting the default column ozone in CMAQ by TOMS data, the modeled J values indicate ozone concentration changes as large as 6%.**

Acknowledgement

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